ACS Sustainable Chemistry & Engineering

Research Article

pubs.acs.org/journal/ascecg

# Full Chain Life Cycle Assessment of Greenhouse Gases and Energy Demand for Canola-Derived Jet Fuel in North Dakota, United States

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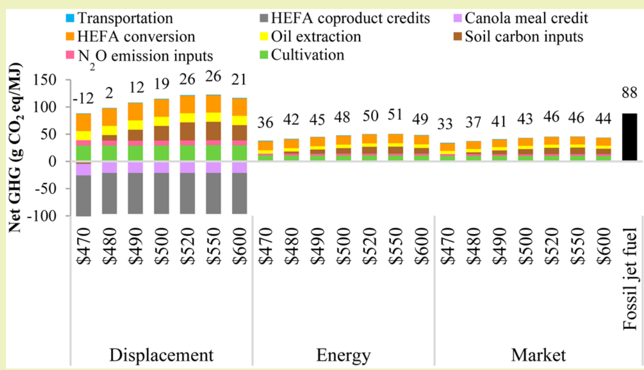
*Supporting Information*

**ABSTRACT:** The success of long-term sustainable biofuel production on agricultural lands is still questionable. To this end, we investigated the effects of crop prices on the changes of agricultural land use for biofuel canola production in three wheat crop management zones in North Dakota. The effects of canola hydroprocessed esters and fatty acids (HEFA) production on greenhouse gas (GHG) emissions and energy demand were investigated along with different allocation methods. The Environmental Policy Integrated Climate (EPIC) and Alternative Fuel Transportation Optimization Tool (AFTOT) models were used to simulate the life cycle assessment (LCA) inputs for two key stages of the HEFA pathway: cultivation and transportation. From the EPIC model results, the increase in canola price had a significant impact on predicted farmer decisions to displace food crops with energy crops and particularly on resulting changes in soil carbon (C). The LCA results suggested that to increase soil C sequestration, energy canola should be grown in the place of the fallow whenever possible to guarantee the long-term soil C sustainability of canola HEFA. Other possible ways to mitigate the GHG emissions included using anhydrous ammonia as the nitrogen fertilizer for cultivation and $H_2$ integration (use of HEFA coproducts in $H_2$ production) for HEFA conversion.




**KEYWORDS:** *Biofuel sustainability, HEFA, Land use change, Canola rotation, EPIC model, AFTOT model*

## INTRODUCTION

**Hydroprocessed Esters and Fatty Acids (HEFA) Fuel.** The International Air Transportation Association (IATA) has established sustainability goals to reduce aviation emissions, which include using 10% renewable fuel by 2017, reducing emissions through carbon neutral growth by 2020, and reducing by 50% the greenhouse gas (GHG) emissions compared to 2005 levels by 2050.[1] Meanwhile, the U.S. Federal Aviation Administration (FAA) has established a goal for the United States aviation fleets to use one billion gallons of renewable jet fuel annually by 2018.[2] HEFA fuel has become important for commercial airlines and the United States aviation fleets since it can be used as a substitute for fossil jet fuel and has the potential to significantly reduce GHG emissions when compared to petroleum jet fuel.[3−6] To achieve these GHG emissions reduction targets will require an advanced knowledge of HEFA pathway emissions and innovations to reduce high emission stages.

**Canola (*Brassica napus*).** Canola is currently considered as a promising feedstock for HEFA since canola provides more oil per hectare than other oilseed crops.[7] In the United States, area used for canola production increased by 36% from $4.65 \times 10^5$ hectares in 2007 to $6.31 \times 10^5$ hectares in 2014. Total canola production increased by 77% from 2007 to 2014.[8,9] Of the

Received: February 7, 2016
Revised: March 25, 2016
Published: April 4, 2016

DOI: 10.1021/acssuschemeng.6b00276
ACS Sustainable Chem. Eng. 2016, 4, 2771−2779

total, 75% of the canola is grown in North Dakota (ND).[8] In the northern plains of ND, canola is typically planted as a rotation crop with small grains (i.e., wheat, barley, oats, and flax),[10] sometimes to replace the fallow period. Growing canola in rotation with wheat provides many advantages over continuous wheat, such as increasing wheat yield, controlling weed problems,[11,12] increasing organic matter in soil, and utilizing deep soil nitrate.[11] However, the production of HEFA fuel from canola has to meet a reduction of 50% in GHG emissions compared to fossil jet fuel in order for canola HEFA fuel to be qualified for the usage mandates of the U.S. EPA's Renewable Fuel Standard (RFS).[13]

**Research Objectives.** There is limited understanding of the effects of bioenergy crop price on changes in various existing food crop rotations to energy crop production for biofuels. This study investigated the effects of energy canola crop price on farmers' decisions to switch from a predominant food cropping system to an energy−food cropping system of canola (energy) in rotation with wheat (food) for HEFA fuel production in the wheat belt in three crop management zones in ND. Specifically, the research objectives are as follows:

- Model GHG emissions, cumulative energy demand (CED), and fossil energy demand (FED) of regional production of HEFA using models of cultivation and supply chain transportation integrated with life cycle assessment (LCA).
- Model effects of canola price on farmers' decisions to switch from a predominantly food cropping system to an energy−food cropping system.
- Incorporate model-based regional inputs for cultivation and transportation into HEFA pathway analysis.
- Interpret LCA results derived from cultivation and transportation models to understand key emission mechanisms.
- Investigate HEFA pathway changes to reduce GHG emissions.

The integration of the Environmental Policy Integrated Climate (EPIC) and Alternative Fuel Transportation Optimization Tool (AFTOT) models was used to simulate regional inputs for cultivation and transportation into the HEFA pathway LCA.

**EPIC Model Description.** The Environmental Policy Integrated Climate (EPIC) model is a biogeochemical-based model originally developed by the U.S. Department of Agriculture and Agriculture Research Service (USDA-ARS).[14] In this study, the EPIC model was used to predict the effects of canola prices (from \$470 to \$600 per Mg of canola seed) on the transition of various existing cropping systems to increase biofuel canola production. The EPIC model simulated the effects of changes in spatial variability in soils, climates, and management decisions of cropping systems of canola−wheat rotation on crop yield, soil carbon change, nutrient requirement, nitrogen (N) loss from nitrate leaching and runoff, and fuel use at farms across geographical regions in ND. Thirty-year simulations were conducted for the most common two-year food crop sequences (i.e., durum−fallow, pea−fallow, spring wheat−spring wheat, spring whea−-pea, spring wheat−sunflower, and spring whea−-winter wheat) observed within each county and for energy crop canola−wheat sequences (canola−spring wheat, canola−winter wheat, and canola−durum). The most common two-year food crop sequences were identified using the USDA-NASS Cropland Data Layer.[15] Simulations were conducted for two tillage systems (no-till and conservation tillage) for each crop sequence on each of the predominant cultivated soil survey geographic database (SSURGO) soil map units[16] within ND. Field management data for each crop sequence and tillage system were constructed based on the USDA-NRCS RUSLE2[17] crop management templates. The daily weather data from January 1981 to December 2010 was acquired from National Climatic Data Center (NCDC), National Oceanic Atmospheric Administration (NOAA).[18] Default values were used for the EPIC model parameters. However, small adjustments were made to crop growth parameters so that average simulated crop yields were within plus or minus 10% of the observed 2002−2012 NASS yields averaged across all counties within each crop management zone. In adjusting crop parameters, management planting and harvest dates were compared to typical planting and harvest dates reported by NASS. Then, potential heat units were adjusted, and heat units at harvest were checked in the model output to make sure that potential heat units were generally just attained each year at the harvest date. Second, the harvest index was adjusted by no more than plus or minus 2%. Finally, if further adjustments were necessary, the maximum leaf area index was adjusted. For the calibration, a simulation was conducted for the dominant cultivated soil type within each county by the EPIC Team at USDA-ARS. Outputs from the EPIC model (canola seed yield, fertilizer use, fuel use, nitrate leaching and runoff, soil C change averaged over 30 years) were input into the LCA on an annual basis.

**AFTOT Model Description.** The Alternative Fuel Transportation Optimization Tool (AFTOT) was developed by the U.S. Department of Transportation (USDOT), John A. Volpe National Transportation Systems Center (Volpe).[19] In this study, the AFTOT model was used to generate the preprocessor origin locations (counties in which canola seed is grown) based on agricultural data obtained from EPIC model and also identified potential biorefinery candidate locations (locations where canola oil is extracted and converted to HEFA fuel) based on the amount of canola oil and HEFA fuel transported. The AFTOT model also optimized routing for moving canola seed from preprocessor to biorefineries and then finally HEFA to Minneapolis−Saint Paul (MSP) airport, based on the lowest transportation and transloading costs, biorefinery capital costs, and minimum and maximum conversion facility capacity. Outputs of AFTOT included the routes, costs, vehicle loads, vehicle miles traveled, $CO_2$ emissions, and fuel consumption for the transport of feedstock and fuel. The assumptions and parameter settings for particular scenarios of transporting feedstock and HEFA fuel (see details in Lewis et al.[19] report) in the AFTOT model were calibrated and validated by the AFTOT Team at Volpe. Fuels and other outputs on an annual basis from AFTOT were input into the LCA, as described below.

## LIFE CYCLE ASSESSMENT METHOD

**Goal and Scope.** The goal and scope of this study are to use the combined outputs from EPIC and AFTOT as well as other LCA inputs from the literature and other sources to determine the sustainability of canola HEFA production over the entire life cycle in terms of GHG emissions, CED, and FED. In addition, alternative allocation methods were employed, for example, displacement, energy, and market allocation methods, in order to address regulatory requirements in different jurisdictions (United States, European Union).



DOI: 10.1021/acssuschemeng.6b00276
ACS Sustainable Chem. Eng. 2016, 4, 2771−2779

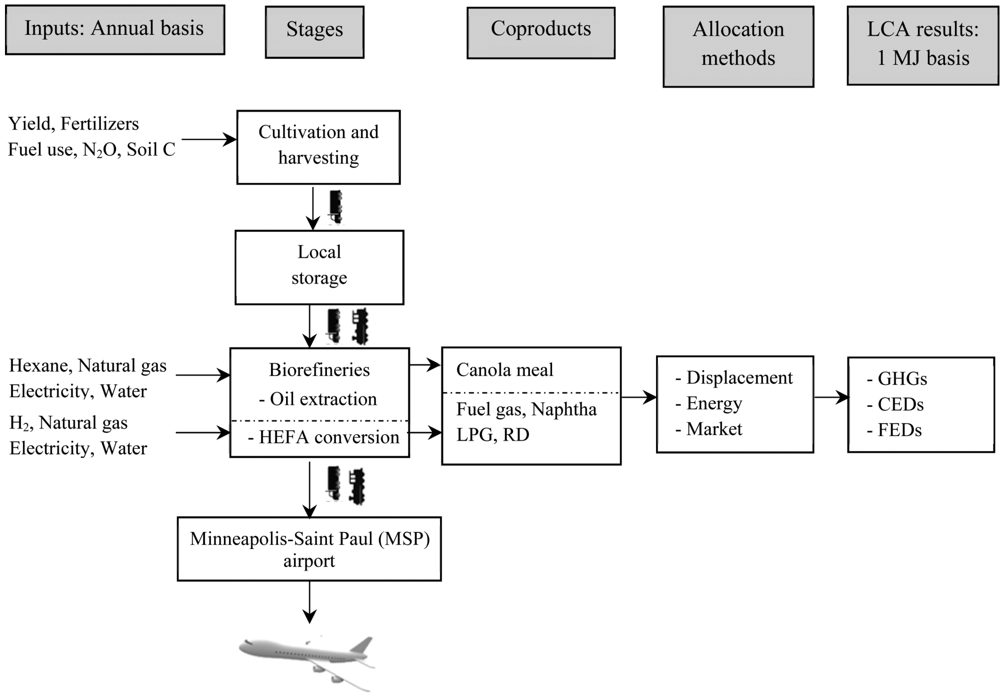



**Figure 1.** System boundary of the canola HEFA fuel pathway.

Sensitivity analyses of N fertilizer type and $H_2$ source were conducted to determine the influence of these factors on the overall GHG emissions of canola HEFA. The geographical areas for canola production were on wheat-growing regions in three crop management zones in ND. Direct land use change (dLUC) emissions were included in this analysis with impacts quantified as the annual change in soil C. Transformation of the existing crops to biofuel production has the potential to impact the indirect land use change (iLUC) $CO_2$ emissions due to other places needing to cultivate food crops for their replacement, in which case the iLUC may increase the final GHG emissions of canola HEFA fuel. However, possible iLUC emissions were excluded from this study due to estimation difficulties for identifying the exact location of iLUC[20] and limitations of the international accounting standards model.[21]

**System Boundary and Functional Unit.** The system boundary of the canola HEFA fuel life cycle is "farm to fly (F2F)", as shown in Figure 1. The fuel pathway starts with cultivation and harvesting of canola. After harvesting, canola seed is transported to local storage on the farm. Then, the canola seed from local storage is transported to biorefineries. At the biorefineries, the canola seed is pressed and extracted with hexane solvent, producing canola meal and canola oil. The canola oil is then processed into canola HEFA fuel at the HEFA conversion unit at the biorefinery. The canola HEFA fuel at the biorefineries is then transported and distributed to the MSP airport as the final destination. The combustion of the HEFA fuel is the final stage of the process. The $CO_2$ emission from HEFA fuel combustion is considered as carbon neutral; therefore, this emission is not counted in the GHG analysis. In this case, the $CO_2$ uptake during cultivation is also not counted. Only fossil $CO_2$ is included plus other greenhouse gases. Different allocation methods were used to evaluate the environmental burdens of coproducts produced from the HEFA fuel: canola meal, fuel gas, naphtha, liquid petroleum gas (LPG), and renewable diesel (RD). The functional unit of the final LCA results is based on 1 MJ of energy content in the HEFA fuel. United States conventional fossil jet fuel is used as the reference fuel, whose GHG emissions, CED, and FED are 88 g $CO_2$ eq/MJ,[22] 1.23 MJ/MJ, and 1.21 MJ/MJ,[6] respectively.

**Coproduct Allocation Methods.** Displacement, energy, and market allocation methods were used to evaluate the effects of the coproducts. For the displacement method, canola meal was assumed to displace soybean meal in the United States, utilizing it as an animal feed. On the basis of on protein content, 1 kg canola was equivalent to 0.87 kg soybean meal.[5] The emission factor for soybean meal was taken to be 460 g $CO_2$ eq/kg dry meal.[23] Meanwhile, fuel gas, liquid petroleum gas (LPG), naphtha, and renewable diesel (RD) were assumed to displace comparable fossil fuels in the market. Cradle-to-gate GHG emissions credits for fuel gas, LPG, naphtha, and RD were obtained from the ecoprofiles in the ecoinvent database.[24] Credits for combustion emissions of the fossil fuels displaced by the coproducts produced from the HEFA conversion process were accounted for based on stoichiometric combustion factors (i.e., 3 kg $CO_2$/kg fuel gas, 3 kg $CO_2$/kg LPG, 3.06 kg $CO_2$/kg naphtha, and 3.17 kg $CO_2$/kg diesel). The lower heating value and market values for product and coproducts for the oil extraction stage were obtained from the GREET model.[3] The energy and market values for the HEFA conversion stage were taken from the GREET model,[3] and Annual Energy Outlook 2015[25] for the petroleum and other liquids price projections in 2020, respectively. The market values for the projection in 2020 were used since we assumed that the HEFA fuel will be commercially available in the next five years and the HEFA price will equal that of fossil jet fuel. The detailed calculations and the values of energy and market allocation factors (AF) applied to the canola oil at the oil extraction stage and canola HEFA at the HEFA conversion stage are provided in Section 1 of the Supporting Information. However, it needs to be noted that each of the allocation methods applied in this study has its limitations. For instance, displacement allocation could give misleading results as it adds considerably high GHG credits to


DOI: 10.1021/acssuschemeng.6b00276
ACS Sustainable Chem. Eng. 2016, 4, 2771−2779

the main product (HEFA) for displacing conventional fossil fuels and animal feed, without considering the interaction with its completing products. Further, it causes concern for market saturation, in which case the value of the coproducts would risk being marginalized, especially in this study the highest price scenario has a 10 times larger production scale than the low price scenarios. For energy allocation, the coproduct maybe mistreated if their energy values do not with certainty affect their emissions in the system. If coproducts are treated by market value allocation, the market values of the final products change over time as the market fluctuates, thus causing varieties of the GHG emission results.

**Life Cycle Inventory Data and Assumptions.** The ecoinvent database V3.0 was used to the generate life cycle inventory (LCI) data for inputs such as those shown in Figure 1 within the LCA software tool SimaPro 8.0. Although, the electricity grid is an interconnected system,[26] the electricity generation for ND was modeled as a mix of United States generation types in ecoinvent according to information in the U.S. EPA eGRID database[27] (Table S.2 Supporting Information). Nonetheless, the sensitivity analysis of electricity was conducted to determine the GHG results with change to the Midwest Reliability Organization (MRO) grid mix profile in the ecoinvent database, as shown in Table S.3 of the Supporting Information. Over the range of oilseed prices and for all allocation methods, the change in net GHG emissions is only 0.5−1.3 g $CO_2$ eq/MJ HEFA, with the ND grid yielding the higher emissions. Farm machinery and plant construction were excluded from the inventory analysis because these effects are normally negligible for these long-lived infrastructure items. The LCI data and assumptions for each stage are described in detail below.

**Cultivation and Other Activities at Farm.** From the EPIC model simulations, canola was modeled as a rotation crop with wheat (see details in Tables S.4−S.6, Supporting Information) for 30 years. It was assumed that farmers will choose the cropping systems that will provide the highest income. As the selling price of canola increases, it is reasonable to expect more farmers to plant canola in order to maximize revenue (see change in food crop production in Table S.7, Supporting Information). Canola seed harvest was assumed to be conducted using a combine harvester with 9% seed moisture content at harvest and 44% oil content, and fuel consumption was modeled by EPIC. After harvesting, canola seed was transferred from a grain-hauling tractor using a diesel-powered auger into a 32 ton truck. A diesel-powered auger use was modeled for transferring canola seed at the field throughout the transportation processes for five steps from (1) grain-hauling tractor to on-farm truck , (2) on-farm truck to local storage (on-farm grain bin or local grain elevator), (3) local storage to long haul trucks, (4) either trucks, rail cars, or barges to biorefinery, and (5) from biorefinery storage to biorefinery facility. It was assumed that each auger step and grain-hauling tractor consumed 0.47 L diesel/Mg canola seed. The upstream emission of diesel production was assigned a value of 0.75 kg $CO_2$ eq/kg diesel based on the conventional diesel United States average in 2005, the most recent year reported.[22] The nitrogen (N) and phosphorus (P) fertilizers were assumed to be the United States average fertilizer mix (see details in Tables S.8 and S.9, Supporting Information)[23] due to lack of information on the specific types of N and P fertilizers used in ND.[28] To determine the direct field $N_2O$ emissions, the emission factor of 0.0035 kg N in $N_2O$/kg N in fertilizer was used since EPIC was not validated yet for $N_2O$ emissions at the time of publication. This $N_2O$ emission value was averaged from the literature data of soil $N_2O$ measurements for canola cultivation in semiarid or dryland regions according to studies by Schwenke et al.[29] and Li et al.[30] (Table S.10, Supporting Information). For indirect $N_2O$ emissions (nitrate leaching/runoff and $NH_3$ volatilization), the EPIC model was used to simulate the annual nitrate leaching and runoff fluxes, whereas the IPCC emission factor was used to estimate $NH_3$ volatilization (0.1 kg N in $NH_3$/kg N input) due to no validation of $NH_3$ volatilization for EPIC. The $N_2O$ emission factor of 0.0075 kg N in $N_2O$/kg $NO_3$−N and 0.01 kg N in $N_2O$/kg $NH_3$−N obtained from the IPCC were applied for nitrate leaching/runoff and volatilized $NH_3$,[31] respectively. The $CO_2$ emission factor from soils due to application of urea fertilizer was estimated as 1.57 kg $CO_2$/kg N in urea based on the fraction of C and N in urea. The annual data inputs for the cultivation stage are provided in Tables S.11 and S.12 of the Supporting Information.

**Oil Extraction (Co-Located at Biorefinery).** Canola seed from multiple local storage sites was modeled as transported to regional biorefineries in ND for conversion to canola oil using the AFTOT model. The transportation details of canola seed from preprocessors to biorefineries are described in the Transportation Section. The amount of wastewater produced from the oil extraction process was assumed from the GREET model to be 0.84 $m^3$/Mg oil.[3] The wastewater treatment of the vegetable oil extraction profile from the ecoinvent database was used in the study, which had the GHG emissions of 1.11 kg $CO_2$ eq/$m^3$ of water treated.[24] The $CO_2$ emissions from the hexane solvent was 3.07 kg $CO_2$/kg hexane, calculated assuming that all hexane emitted to the environment is oxidized to $CO_2$. The annual inputs for the oil extraction stage are provided in Table S.13 of the Supporting Information.

**HEFA Conversion (Located at Biorefinery).** The data inputs and outputs of the HEFA conversion were taken from pennycress-derived jet fuel (obtained from UOP), and were assumed to be valid for the conversion of canola oil to HEFA.[6] This assumption is reasonable since the unsaturated fatty acid profile of canola oil (56 wt % monounsaturated, 26 wt % dual unsaturated, and 10 wt % triple unsaturated)[32] are close to field pennycress oil (56 wt % monounsaturated, 25 wt % dual unsaturated, and 12 wt % triple unsaturated),[33] resulting in similar $H_2$ consumption for the hydrogenation process to saturate these bonds. Pennycress is a winter annual crop that is currently being developed as an oilseed crop for biofuel production in the U.S.[34] In the Honeywell's UOP Ecofining process for renewable diesel (RD) and renewable jet (HEFA) hydroconversion process, canola oil input of 2.101 Mg is required to produce 1 Mg of canola HEFA fuel. The low HEFA yield is due to the coproduction of a suite of hydrocarbon renewable fuels. $H_2$, electricity, and natural gas were the major inputs for the HEFA conversion stage. The $H_2$ source was assumed to be produced from natural gas via steam methane reforming, which was modeled in ecoinvent based on UOP data with emission factor of 13.3 kg $CO_2$ eq/kg $H_2$. According to the ecoinvent, the $CH_4$ emission rate from upstream natural gas was 0.114 g $CO_2$ eq/MJ natural gas. Although, the data inputs for the HEFA conversion were confidential UOP data which cannot be shown, we provide similar inputs and outputs for the HEFA conversion process based on a published Stratton[35] study (see Supporting Information, Table S.14).



DOI: 10.1021/acssuschemeng.6b00276
ACS Sustainable Chem. Eng. 2016, 4, 2771−2779

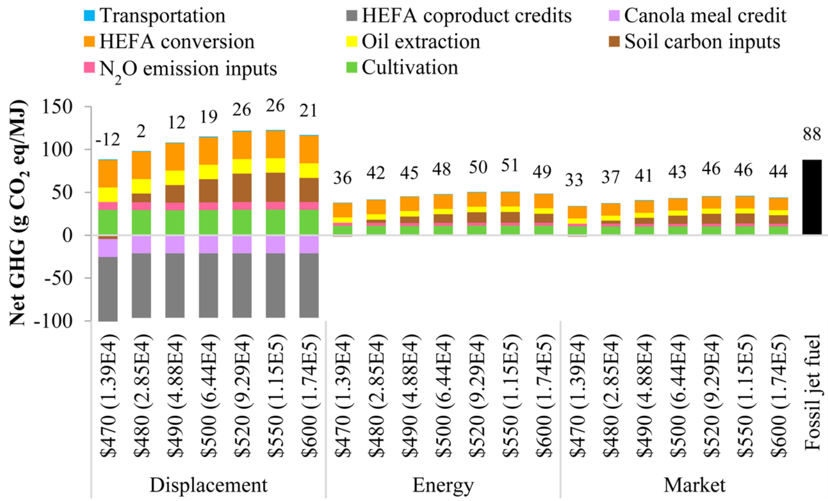



**Figure 2.** GHG emissions of canola HEFA at different prices along with different allocation methods compared to fossil jet fuel.

**Transportation.** It was assumed that a truck transported canola seed from the field to local storage with an average distance of 4 km. Key inputs for the biomass supply and biofuel distribution were obtained from the AFTOT model. The main transportation pathways simulated using the AFTOT model included transporting canola seed from the local storages to biorefinery candidate locations with either trucks, rail cars, or barges, and transporting canola HEFA fuel between biorefineries and the MSP airport with either trucks, rail cars, barges, or by pipeline. The upstream emission of diesel production was 0.75 kg $CO_2$ eq/kg diesel.[22] The details of the transportation data and transportation maps are provided in Tables S.15−S.17 and Figures S.4−S.10 of the Supporting Information.

**Life Cycle Impact Assessment.** The SimaPro 8.0 software[36] was used to evaluate the GHG emissions, CED, and FED of the canola HEFA fuel. The IPCC 2013 GWP 100a V1.00 and the CED V1.08 methods were used to calculate the GHG emissions and the energy demand, respectively. The main sources of GHG emissions considered were $CO_2$, $CH_4$, and $N_2O$, whose 100-year global warming potentials are 1, 28, and 265, respectively,[36] but all greenhouse gases included in ecoprofiles used were added to the GWP analysis. In this study, the GWP values were obtained from the IPCC method used in SimaPro 8.0 and not the most recent GWP value for $CH_4$ from the 2013 IPCC reports.

## RESULTS

**GHG Emissions of Canola HEFA Life Cycle.** Figure 2 displays the GHG emissions of the canola HEFA fuel life cycle over the price ranges from \$470−\$600 per Mg seed. Different coproduct allocation methods are included with a comparison to fossil jet fuel. The net GHG emissions are presented as numbers above each bar. The amount of HEFA production (Mg/yr), calculated based on UOP HEFA yield data, for each price is shown in parentheses in Figure 2. The GHG emissions of canola HEFA fuel for each stage are provided in Table S.18 of the Supporting Information.

The results showed that the trends of the GHG emissions were similar for all allocation methods, with the GHG emissions increasing with increased canola seed price to a maximum at \$550 and then decreasing slightly until \$600. These variations of GHG emissions were mainly from soil C change predicted by the EPIC model. Key stages for emissions include HEFA production ($H_2$), soil C change, and cultivation (N fertilizer), while secondary in importance are oil extraction (natural gas and electricity), $N_2O$ emissions, and transportation (diesel fuel). The activities in parentheses represent the key contributors within each stage. Credits in emissions for displacement allocation are dominated by coproducts from the HEFA stage and canola seed meal from oil extraction.

Soil C change was the only factor influenced by canola seed price due to the transition of agricultural land use, which caused either an emissions benefit or disadvantage for the canola HEFA fuel. The GHG emissions of soil C change showed a decrease of −4.4 g $CO_2$ eq/MJ at the price of \$470 due to soil C sequestration from replacing the fallow cropping systems of durum−fallow and pea−fallow by a canola−spring wheat rotation. However, some of this C sequestration was offset as some sunflower−spring wheat area was also replaced by canola−spring wheat. For prices of \$480−\$550, more canola production occurred in place of existing crops, including corn, durum, and sunflower, resulting in decreases in soil C due to lower soil C inputs from canola residue compared to residues from these displaced crops. However, as price increased to \$600, loss of soil C decreased since canola began to displace more soybean, which has lower soil C inputs from roots and residues. As the price increased, the canola feedstock and number of counties participating increased, resulting in an increase in HEFA production. Consequently, the transportation required to move canola feedstock and HEFA fuel increased. However, transportation GHG emissions per MJ HEFA increased only slightly over the price range, as shown in Table S.18 of the Supporting Information, suggesting that the locations of the biorefineries determined from the AFTOT model kept emissions and costs for transportation from rising significantly. The results indicated that the displacement allocation method showed the most favorable results of GHG emissions among all methods due to taking into account the GHG emission credits from canola meal and HEFA coproducts. It was observed that the GHG results generated using the market method were slightly lower than that from the energy method due to a higher market price for HEFA coproducts than HEFA fuel (Table S.1, Supporting Information). However, it is important to note that the results of the GHG emissions generated using the market method could change over time depending on the market price of products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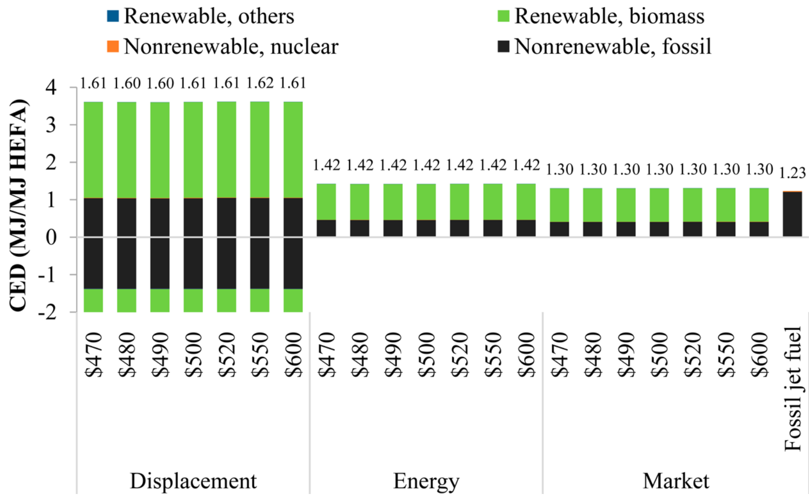


**Figure 3.** Total CED of canola HEFA at different prices along with different allocation methods compared to fossil jet fuel.

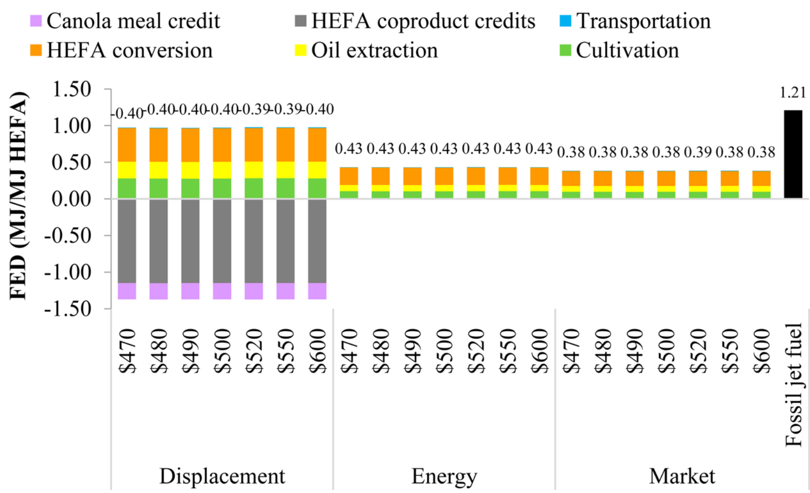


**Figure 4.** Total FED of canola HEFA at different prices along with different allocation methods compared to fossil jet fuel.

(Figure S.3, Supporting Information). Overall, the GHG emissions of canola HEFA over the price range from \$470 to \$600 using the displacement allocation method exhibited GHG savings ranging from 70% to 114%. However, the canola HEFA from some of the prices for energy and market methods failed to meet 50% GHG savings compared to fossil jet fuel. Nonetheless, it should be noted that the baseline fossil jet fuel is representative of only one type of coproduct allocation method (energy method[22]), which is not directly comparable to all scenarios. Specifically, the displacement scenario results are compared with those of the baseline fossil jet fuel that do not use the displacement method.

**Cumulative Energy Demand (CED) of Canola HEFA.** Figure 3 shows the CED of canola HEFA fuel at different prices compared to fossil jet. The types of energy demands for producing canola HEFA were composed of four major categories: nonrenewable fossil, nonrenewable nuclear, renewable biomass, and renewable others (i.e., wind, solar, geothermal, and water). The CED of canola HEFA fuel for each stage are provided in Table S.19 of the Supporting Information.

The results indicated that the canola HEFA fuel demanded more energy than fossil jet fuel. However, the sources of energy demand for producing the canola HEFA fuel were mainly from renewable biomass for all allocation cases. Thus, the canola HEFA fuel required less fossil energy compared to fossil jet fuel. The results of CED generated using market allocation were lower than energy allocation since the market allocation factor (Table S.1, Supporting Information) at the oil extraction and HEFA conversion stages was lower than the energy allocation factor.

**Fossil Energy Demand (FED) of Canola HEFA Fuel.** Figure 4 shows the FED for each stage of the canola HEFA fuel at different prices compared with FED for fossil jet fuel. The total FED results of the canola HEFA fuel at each stage are provided in Table S.20 of the Supporting Information. The results showed that the canola HEFA fuel required lower fossil energy demand than fossil jet fuel for all cases. The displacement method showed the most favorable results of FED because of the credit provided by coproducts from oil extraction and HEFA conversion, which significantly reduced the fossil energy demand for the canola HEFA fuel. Canola cultivation was the most energy-intensive stage for the displacement method due to the use of energy associated with the N fertilizer production process. On the other hand, the HEFA conversion process exhibited the largest contribution of FED for the energy and market methods due to energy consumption associated with $H_2$ produced from natural gas. The fossil energy demand from the transportation stage was


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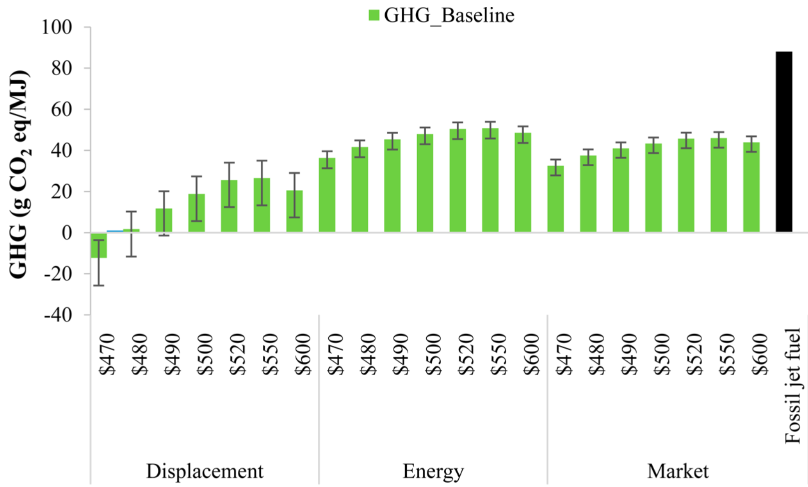


**Figure 5.** Influence of N fertilizer types on the GHG emissions of canola HEFA for natural gas $H_2$.

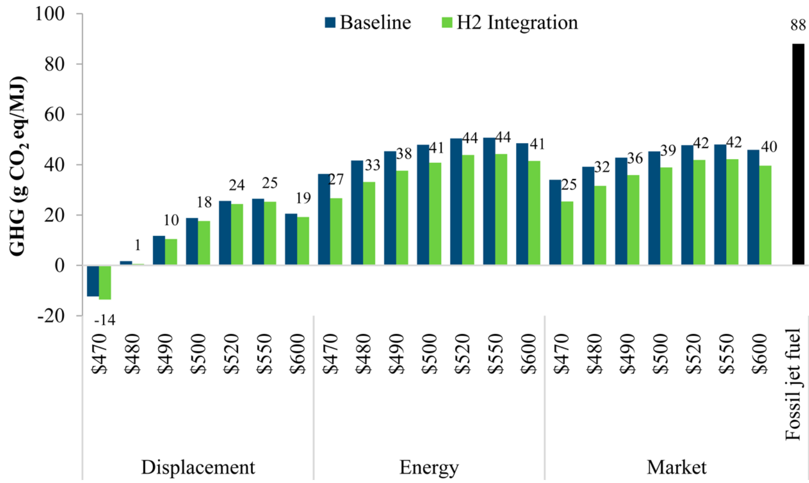


**Figure 6.** GHG emissions of canola HEFA fuel for the $H_2$ integration scenario compared to GHG emissions from baseline HEFA. Total values for the $H_2$ integration scenario are shown to demonstrate achievement of 50% GHG reduction compared to petroleum jet fuel.

relatively small compared to other stages, approximately 1% of the FED for canola HEFA.

**Sensitivity Analysis.** *Alternative N Fertilizer Choices during Cultivation Stage.* From the baseline results above, the production of the United States mix of N fertilizer was the main GHG emissions contributor for the cultivation stage. In this section, scenario analyses were conducted to estimate the range of GHG emissions regarding different types of N fertilizer as affected by the N production process and $NH_3$ volatilization emitted on dryland regions (see details in Section S.3, Supporting Information). Four common types of N fertilizers, urea, urea ammonium nitrate (UAN), ammonium sulfate (AS), and anhydrous ammonia (AA), were chosen. Ammonium nitrate (AN) was excluded because it is generally no longer commercially available in the ND area due to security concerns.[37] Sensitivity analysis results for N fertilizer types on the GHG emissions of canola HEFA are shown in Figure 5. Error bars represent the GHG variations of the lowest emission (using ammonium sulfate as N fertilizer) and highest emission scenarios (using urea ammonium nitrate as N fertilizer).

Results indicated that N fertilizer types have a significant impact on the overall GHG emissions of canola HEFA fuel over the price range. The highest emissions would be a result of using UAN, with GHG increases of 8.5, 3.1, and 2.9 g $CO_2$ eq/MJ for the displacement, energy, and market cases, respectively. On the other hand, using AS as the N fertilizer showed GHG reductions of 13.2, 4.9, and 4.6 g $CO_2$ eq/MJ for the displacement, energy, and market cases, respectively. However, considering the relatively high sulfur content in ammonium sulfate, which could possibly load the soil with too much S, anhydrous ammonia would be a better option when choosing N fertilizer in a GHG perspective, with only a small amount of increased GHG emissions over ammonium sulfate. From the results, all price points could meet the 50% reduction if using AA as the primary N fertilizer source.

*$H_2$ Source for HEFA Conversion Stage.* From the baseline results, $H_2$ was the main contribution to the GHG emissions of the HEFA conversion stage due to its production from natural gas via the steam methane reforming process. However, the low molecular weight hydrocarbon coproducts obtained from the HEFA conversion could be used to produce the $H_2$. A sensitivity analysis of $H_2$ production from HEFA coproducts was conducted in order to investigate the influence of $H_2$ sources on GHG emissions of canola HEFA. For this scenario ($H_2$ integration), $H_2$ was assumed to be produced from fuel gas, LPG, and some smaller amounts of naphtha, instead of natural gas. Additional inputs for $H_2$ plant utilities included electricity, boiler feedwater, and cooling water (confidential UOP

Honeywell) were added. The GHG emissions results of canola HEFA for the $H_2$ integration scenario compared to the baseline GHG results are shown in Figure 6. The values of energy and market allocation factors for $H_2$ integration are provided in Table S.23 of the Supporting Information.

From the results, a decrease in GHG emissions of canola HEFA over the price range was found when the $H_2$ integration was combined with the HEFA conversion stage. These results show that the use of integrated $H_2$ achieves a 50% savings of GHG emissions compared to fossil jet for all oilseed price points, a significant improvement over the base case results.

## DISCUSSION

The full chain life cycle assessment for GHG emissions and energy demand for the canola HEFA fuel in three crop management zones in ND was conducted using a field-scale cultivation model, a supply chain transportation model with different allocation methods, and scenarios on important pathway assumptions. On the basis of the results, it can be concluded that changes in canola prices significantly impacted predicted transitions of agricultural land use in ND. These transitions had a large influence on the canola farming impacts and particularly changes in soil C, a main factor which could be a GHG benefit or disadvantage for canola HEFA. The land use changes were much more complex than a simple substitution of canola production for one particular crop. However, it is recognized that many other factors can influence land use decisions besides crop price. The results from the LCA analysis suggested that to increase soil C sequestration, canola should be grown in place of fallow where possible in order to guarantee the long-term soil C sustainability of canola HEFA. Other possible ways to mitigate the GHG emissions included switching from a United States fertilizer mix to anhydrous ammonia and changing the $H_2$ source of HEFA conversion from natural gas to low molecular weight HEFA coproducts.

However, there were limitations in this LCA analysis. The EPIC model has a limitation in simulating changes in direct $N_2O$ emissions and indirect $N_2O$ from $NH_3$ volatilization for the transition of agricultural land use. The current version of EPIC greatly overpredicted $N_2O$ emissions compared to field measurements from dry land cropping, and therefore, an average of the literature data was used instead. Moreover, this study excluded the changes in direct $N_2O$ emissions from changes in crop residue input to the soil due to limitations in the current EPIC version. Furthermore, our study excluded the indirect LUC analysis due to its high uncertainty, although we recognize the potential for iLUC effects from the net decrease in food production predicted by the EPIC model (Table S.7, Supporting Information). To improve the EPIC model, soil measurement data of both direct $N_2O$ emissions and $NH_3$ volatilization at different field sites are needed to estimate and validate model parameters. The other areas needed to improve the LCA analysis include analysis of the iLUC, use of specific data for the canola upgrading profile, continued enhancement of local-level realism of the AFTOT model, and inclusion of other sustainability indicators such as erosion, water footprint, nutrient runoff, and change in fertilizer use in the model region.

Despite the limitations mentioned, there are a number of advantages in the modeling approach to predict sustainability of future biofuel production. This study investigated the effects of energy crop price on farmers' decisions; effects of decisions on soil sustainability metrics, such as soil carbon and nutrient cycling, on optimum location of biorefineries, minimum supply chain cost, and fuel consumption, as well as impacts of LCA assumptions with regard to allocation, N fertilizer type, and $H_2$ source. The modeling approach is suitable for building a more comprehensive set of LCA indicators to improve predictions and guide sustainable biofuel development in energy−food coproduction cultivation systems.

## ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acssuschemeng.6b00276.

> Calculation of energy and market allocation factor (AF); Electricity resources mix for North Dakota state; GHG emissions results for changing electricity generation from ND electricity resource mix to the Midwest Reliability Organization (MRO) grid mix; Canola−wheat rotation: plant schedules; Change in food crop production at different canola prices; Nitrogen and phosphorus fertilizer mixtures; Emission factor of N apply for canola cultivation in semiarid and dryland regions; Annual data inputs for canola farming, oil extraction, HEFA conversion, and transportation stages; GHG emissions, CED, and FED of canola HEFA fuel over the price range for the displacement, energy, and market allocation methods; GHG emissions of canola HEFA fuel for using different N fertilizer types; GHG emissions of canola HEFA fuel for $H_2$ integration scenario; GHG emissions of canola HEFA fuel for using different United States fuel prices for market value allocation; Transportation map for canola price \$470−\$600. (PDF)

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### Notes

The authors declare no competing financial interest.

## ACKNOWLEDGMENTS

Funding from the Michigan Tech subaward No. 59-3620-3-002 and USDA-ARS Interagency Agreement No. 60-3620-2-361/ USDA-NIFA-BRDI # 2012-10008-19727 is appreciated. Volpe development of AFTOT was funded by the Federal Aviation Administration (FAA) and Office of Naval Research under Interagency Agreement No. DTFAVP-12-X-00177 and by the FAA under Agreement Nos. DTFAVP-14-X-00118 and DTFAVP-15-X-00097. We thank UOP (a Honeywell Company) for HEFA conversion data.

## REFERENCES

(1) IATA Technology Roadmap, 2013. International Air Transport Association. http://www.iata.org/whatwedo/environment/Documents/technology-roadmap-2013.pdf (accessed April 14, 2015).

(2) Sustainable Alternative Jet Fuels. Federal Aviation Administration. https://www.faa.gov/about/office_org/headquarters_offices/apl/research/alternative_fuels/ (accessed August 18, 2015).

(3) Wang, M. *GREET1_2014 Transportation Fuel-Cycle Model*; Center for Transportation Research, Energy Systems Division, Argonne National Laboratory: Argonne, IL, 2014.

(4) Shonnard, D. R.; Williams, L.; Kalnes, T. N. Camelina-derived jet fuel and diesel: Sustainable advanced biofuels. *Environ. Prog. Sustainable Energy* **2010**, *29* (3), 382−392.

(5) Stratton, R. W.; Wong, H. M.; Hileman, J. I. *Life Cycle Greenhouse Gas Emissions from Alternative Jet fuels*; Partnership for Air Transportation Noise and Emissions Reduction (PARTNER) Report Number 2010-001; Massachusetts Institute of Technology: Cambridge, MA, 2010. http://web.mit.edu/aeroastro/partner/reports/proj28/partner-proj28-2010-001.pdf (accessed October 10, 2012).
(6) Fan, J.; Shonnard, D. R.; Kalnes, T. N.; Johnsen, P. B.; Rao, S. A life cycle assessment of pennycress (Thlaspi arvense L.)-derived jet fuel and diesel. *Biomass Bioenergy* **2013**, *55*, 87−100.
(7) Collins, H. P.; Boydston, R.; Alva, A. Biofuel Variety Trials. U.S. Department of Agriculture. http://www.pacificbiomass.org/documents/OilSeed/BiofuelsVarietyTrialsHalCollins.pdf (accessed August 18, 2011).
(8) Crop Production 2014 Summary, 2015. U.S. Department of Agriculture, National Agricultural Statistics Service. http://www.usda.gov/nass/PUBS/TODAYRPT/cropan15.pdf (accessed August 18, 2015).
(9) 2007 Census of Agriculture, 2007. U.S. Department of Agriculture, National Agricultural Statistics Service. http://www.agcensus.usda.gov/Publications/2007/Full_Report/Volume_1,_Chapter_1_US/st99_1_033_033.pdf (accessed August 18, 2015).
(10) Soybeans & Oil Crops: Canola, 2012. U.S. Department of Agriculture, Economic Research Service. http://www.ers.usda.gov/topics/crops/soybeans-oil-crops/canola.aspx (accessed August 18, 2015).
(11) Brown, J.; Davis, J. B.; Lauver, M.; Wysocki, D. U.S. Canola Growers' Manual, 2008. U.S. Canola Association. http://www.uscanola.com/site/files/956/102387/363729/502632/Canola_Grower_Manual_FINAL_reduce.pdf (accessed August 5, 2013).
(12) Boyles, M.; Peeper, T.; Stamm, M. Great Plains Canola Production Handbook, 2009. http://canola.okstate.edu/ocesfactsheets/canolaproductionhandbook2009.pdf (accessed June 5, 2013).
(13) Renewable Fuel Standard. EPA Issues Direct Final Rule for Additional Qualifying Renewable Fuel Pathways under the RFS2 Program, 2011; EPA-420-F-1-−04;, U.S. Environmental Protection Agency. http://www.epa.gov/sites/production/files/2015-08/documents/420f11043.pdf (accessed August 10, 2013).
(14) Williams, J. R.; Jones, C. A.; Dyke, P. T. A modeling approach to determining the relationship between erosion and soil productivity. *Trans. ASAE* **1984**, *27*, 129−144.
(15) Cropscape-Cropland Data Layer. U.S. Department of Agriculture, National Agricultural Statistics Service. http://nassgeodata.gmu.edu/CropScape (accessed April 29, 2014).
(16) Soil Survey Staff Gridded Soil Survey Geographic (SSURGO) Database for the Conterminous United States. U.S. Department of Agriculture, National Agricultural Statistics Service. https://gdg.sc.egov.usda.gov/ (accessed October 7, 2014).
(17) RUSLE2 Crop Management Templates. U.S. Department of Agriculture, Natural Resources Conservation Service. http://www.nrcs.usda.gov/wps/portal/nrcs/detail/national/technical/tools/rusle2/?cid=stelprdb1247555 (accessed February 20, 2014).
(18) Climate Data Online Search. National Oceanic and Atmospheric Administration, National Climatic Data Center. http://www.ncdc.noaa.gov/ (accessed September 3, 2014).
(19) Lewis, K. C.; Baker, G. M.; Pearlson, M. N.; Gillham, O.; Smith, S.; Costa, S.; Herzig, P. *Alternative Fuel Transportation Optimization Tool: Description, Methodology, and Demonstration Scenarios*; Report Number DOT-VNTSC-FAA-1-−11; U.S. Department of Transportation, John A. Volpe National Transportation Systems Center: Cambridge, MA, 2015. http://ntl.bts.gov/lib/56000/56200/56200/Alt_Fuel_Trn_Optimization_Tool.pdf (accessed October 20, 2015).
(20) Bourguignon, D. EU Biofuels Policy: Dealing with Indirect Land Use Change, 2015. European Parliament. http://www.europarl.europa.eu/RegData/etudes/BRIE/2015/548993/EPRS_BRI(2015)548993_REV1_EN.pdf (accessed March 14, 2016).
(21) Finkbeiner, M. Indirect land use change − Help beyond the hype? *Biomass Bioenergy* **2014**, *62*, 218−221.
(22) *Development of Baseline Data and Analysis of Life Cycle Greenhouse Gas Emissions of Petroleum-Based Fuels*; Report Number DOE/NETL-2009/1346; National Energy Technology Laboratory, U.S. Department of Energy. http://www.netl.doe.gov/energy-analyses/pubs/NETL%20LCA%20Petroleum-based%20Fuels%20Nov%202008.pdf (accessed November 26, 2013).
(23) Adom, F.; Maes, A.; Workman, C.; Clayton-Nierderman, Z.; Thoma, G.; Shonnard, D. Regional carbon footprint analysis of dairy feeds for milk production in the USA. *Int. J. Life Cycle Assess.* **2012**, *17* (5), 520−534.
(24) Ecoinvent database V3.0, Swiss Center for Life Cycle Inventories. ecoinvent. http://www.ecoinvent.org/database/ (accessed April 2016).
(25) *Annual Energy outlook 2015 with Projections to 2040*; Report Number DOE/EIA-0383(2015); Energy Information Administration, U.S. Department of Energy: Washington, DC, 2015. http://www.eia.gov/forecasts/aeo/ (accessed October 10, 2015).
(26) Weber, C. L.; Jaramillo, P.; Marriott, J.; Samaras, C. Life Cycle Assessment and Grid Electricity: What Do We Know and What Can We Know? *Environ. Sci. Technol.* **2010**, *44* (6), 1895−1901.
(27) eGRID, 9th ed., Version 1.0, Year 2010 Summary Tables; 2014. http://cityofdavis.org/home/showdocument?id=4349 (accessed April 2016).
(28) Fertilizer Consumption and Use by Year, Table 4: U.S. Consumption of Selected Nitrogen Materials, 1960−2011. U.S. Department of Agriculture, Economic Research Service. http://www.ers.usda.gov/datafiles/Fertilizer_Use_and_Price/Fertilizer_Consumption_and_UseBy_Year_/table4.xls (accessed August 28, 2014).
(29) Schwenke, G.; Haigh, B.; McMullen, G.; Herridge, D., Soil Nitrous Oxide Emissions under Dryland N-Fertilised Canola and $N_2$-Fixing Chickpea in the Northern Grains Region, Australia. In *2010 19th World Congress of Soil Science, Soil Solutions for a Changing World*, Brisbane, Australia, 2010.
(30) Li, C.; Hao, X.; Blackshaw, R. E.; O'Donovan, J. T.; Harker, K. N.; Clayton, G. W. Nitrous oxide emissions in response to ESN and urea, herbicide management and canola cultivar in a no-till cropping system. *Soil Tillage Res.* **2012**, *118*, 97−106.
(31) Klein, C. D.; Novoa, R. S. A.; Ogle, S.; Smith, K. A.; Rochette, P.; Wirth, T. C.; McConkey, B. G.; Mosier, A.; Rypdal, K. *2006 IPCC Guidelines for National Greenhouse Gas Inventories* 2006; p 54.
(32) Gunstone, A. F. Typical Fatty-Acid Compositions of Some Common Fats. web.pdx.edu/~wamserc/C336S12/fat.pdf (accessed September 21, 2015).
(33) Moser, B. R.; Knothe, G.; Vaughn, S. F.; Isbell, T. A. Production and Evaluation of Biodiesel from Field Pennycress (Thlaspi arvense L.) Oil. *Energy Fuels* **2009**, *23* (8), 4149−4155.
(34) Evangelista, R. L.; Isbell, T. A.; Cermak, S. C. Extraction of pennycress (Thlaspi arvense L.) seed oil by full pressing. *Ind. Crops Prod.* **2012**, *37* (1), 76−81.
(35) Stratton, R. W. *Life Cycle Assessment of Greenhouse Gas Emissions and Non-$CO_2$ Combustion Effects from Alternative Jet Fuels*. Master thesis, Massachusetts Institute of Technology, Cambridge, MA, 2010.
(36) *SimaPro, version 8.0*; PRé Consultant: Amersfoort, The Netherlands, 2014.
(37) Ammonium Nitrate Security. U.S. Department of Justice, Bureau of Alcohol, Tobacco, Firearms and Explosives. https://www.atf.gov/explosives/ammonium-nitrate-security (accessed November 20, 2015).


DOI: 10.1021/acssuschemeng.6b00276
ACS Sustainable Chem. Eng. 2016, 4, 2771−2779